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**Density Functional Theory Study of the Multimode Jahn-Teller Problem in the Fullerene Anion**

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# SUPPLEMENTARY INFORMATION

**List of supplementary tables:**

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TABLE S2 Analysis of the multimode JT problem of $C_{60}^{-}$ in $D_{3d}$ conformation by the LS totally symmetric normal modes in the harmonic approximation, IDP analysis at HS point, and the origin of the LS normal modes relative to the HS normal modes.

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TABLE S4 Analysis of the multimode JT problem of $C_{60}^{-}$ in $C_{2h}$ conformation by the LS totally symmetric normal modes in the harmonic approximation, IDP analysis at HS point, and the origin of the LS normal modes relative to the HS normal modes.

**Table S1:** Analysis of the multimode JT problem of $C_{60}^{-}$ in $D_{5d}$ conformation by the LS totally symmetric modes in the harmonic approximation. Frequencies ($\nu_k$) of the selected normal modes are in cm$^{-1}$ as obtained from DFT calculations. The contributions of the normal mode to the JT distortion ($c_k$) and the energy stabilization ($E_k$) are given in %. The origin of the LS normal mode relative to the HS normal mode is given.

| **LS Irrep** | $^{2}A_{2u}$ ($D_{5d}$) $\nu_k$ | $c_k$ | $E_k$ | **Origin of the Irrep** |
|---|---|---|---|---|
| $a_{1g}$ | 260 | 30.14 | 4.87 | $h_g$ #1 |
| $a_{1g}$ | 419 | 40.71 | 17.09 | $h_g$ #2 |
| $a_{1g}$ | 500 | 0.08 | 0.05 | $a_g$ #1 |
| $a_{1g}$ | 708 | 13.03 | 15.63 | $h_g$ #3 |
| $a_{1g}$ | 788 | 4.80 | 7.15 | $h_g$ #4 |
| $a_{1g}$ | 1125 | 1.96 | 5.94 | $h_g$ #5 |
| $a_{1g}$ | 1268 | 0.87 | 3.37 | $h_g$ #6 |
| $a_{1g}$ | 1455 | 5.21 | 26.41 | $h_g$ #7 |
| $a_{1g}$ | 1511 | 0.03 | 0.14 | $a_g$ #2 |
| $a_{1g}$ | 1595 | 3.17 | 19.35 | $h_g$ #8 |

**Table S2:** Analysis of the multimode JT problem of $C_{60}^{-}$ in $D_{3d}$ conformation by the LS totally symmetric modes in the harmonic approximation. Frequencies ($\nu_k$) of the selected normal modes are in $cm^{-1}$ as obtained from DFT calculations. The contributions of the normal mode to the JT distortion ($c_k$) and the energy stabilization ($E_k$) are given in %. The origin of the LS normal mode relative to the HS normal mode is given.

| **LS** | $^{2}A_{2u}$ **($D_{3d}$)** | | | **Origin of the Irrep** |
|---|---|---|---|---|
| **Irrep** | $\nu_k$ | $c_k$ | $E_k$ | |
| $a_{1g}$ | 264 | 36.68 | 6.47 | $h_g$ #1 |
| $a_{1g}$ | 428 | 36.25 | 16.81 | $h_g$ #2 |
| $a_{1g}$ | 477 | 0.46 | 0.26 | $g_g$ #1 |
| $a_{1g}$ | 503 | 0.04 | 0.03 | $a_g$ #1 |
| $a_{1g}$ | 571 | 0.00 | 0.00 | $g_g$ #2 |
| $a_{1g}$ | 707 | 11.69 | 14.85 | $h_g$ #3 |
| $a_{1g}$ | 744 | 0.02 | 0.02 | $g_g$ #3 |
| $a_{1g}$ | 789 | 4.32 | 6.81 | $h_g$ #4 |
| $a_{1g}$ | 1116 | 0.31 | 0.99 | $h_g$ #5, $g_g$ #4 |
| $a_{1g}$ | 1125 | 1.72 | 5.53 | $g_g$ #4, $h_g$ #5 |
| $a_{1g}$ | 1273 | 0.62 | 2.55 | $h_g$ #6 |
| $a_{1g}$ | 1326 | 0.02 | 0.09 | $g_g$ #5 |
| $a_{1g}$ | 1461 | 4.73 | 25.57 | $h_g$ #7 |
| $a_{1g}$ | 1511 | 0.04 | 0.23 | $a_g$ #2 |
| $a_{1g}$ | 1518 | 0.00 | 0.00 | $g_g$ #6 |
| $a_{1g}$ | 1586 | 3.10 | 19.78 | $h_g$ #8 |

**Table S3:** Analysis of the multimode JT problem of $C_{60}^{-}$ in $D_{2h}$ conformation by the LS totally symmetric modes in the harmonic approximation. Frequencies ($\nu_k$) of the selected normal modes are in $cm^{-1}$ as obtained from DFT calculations. The contributions of the normal mode to the JT distortion ($c_k$) and the energy stabilization ($E_k$) are given in %. The origin of the LS normal mode relative to the HS normal mode is given.

| LS | $^2B_{1u}$ ($D_{2h}$) | | | | $^2B_{2u}$ ($D_{2h}$) | | | | $^2B_{3u}$ ($D_{2h}$) | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| irrep | $\nu_k$ | $c_k$ | $E_k$ | Origin | $\nu_k$ | $c_k$ | $E_k$ | Origin | $\nu_k$ | $c_k$ | $E_k$ | Origin |
| $a_g$ | 260 | 18.36 | 2.99 | $h_g$ #1 | 261 | 17.47 | 2.82 | $h_g$ #1 | 261 | 12.32 | 1.98 | $h_g$ #1 |
| $a_g$ | 263 | 12.16 | 2.03 | $h_g$ #1 | 262 | 13.45 | 2.18 | $h_g$ #1 | 263 | 18.29 | 2.99 | $h_g$ #1 |
| $a_g$ | 423 | 20.43 | 8.84 | $h_g$ #2 | 423 | 29.57 | 12.53 | $h_g$ #2 | 426 | 39.30 | 16.84 | $h_g$ #2 |
| $a_g$ | 432 | 19.75 | 8.85 | $h_g$ #2 | 433 | 9.69 | 4.30 | $h_g$ #2 | 430 | 0.77 | 0.34 | $h_g$ #2 |
| $a_g$ | 482 | 0.22 | 0.12 | $g_g$ #1 | 482 | 0.00 | 0.00 | $g_g$ #1 | 482 | 0.04 | 0.02 | $g_g$ #1 |
| $a_g$ | 502 | 0.01 | 0.01 | $a_g$ #1 | 501 | 0.02 | 0.01 | $a_g$ #1 | 502 | 0.00 | 0.00 | $a_g$ #1 |
| $a_g$ | 572 | 0.01 | 0.01 | $g_g$ #2 | 572 | 0.01 | 0.01 | $g_g$ #2 | 572 | 0.00 | 0.00 | $g_g$ #2 |
| $a_g$ | 706 | 3.84 | 4.62 | $h_g$ #3 | 706 | 5.08 | 5.99 | $h_g$ #3 | 706 | 11.30 | 13.37 | $h_g$ #3 |
| $a_g$ | 707 | 9.24 | 11.14 | $h_g$ #3 | 708 | 8.22 | 9.79 | $h_g$ #3 | 707 | 1.62 | 1.92 | $h_g$ #3 |
| $a_g$ | 753 | 0.01 | 0.01 | $g_g$ #3 | 753 | 0.01 | 0.02 | $g_g$ #3 | 753 | 0.01 | 0.02 | $g_g$ #3 |
| $a_g$ | 788 | 5.03 | 7.51 | $h_g$ #4 | 787 | 5.02 | 7.39 | $h_g$ #4 | 788 | 4.96 | 7.29 | $h_g$ #4 |
| $a_g$ | 791 | 0.00 | 0.00 | $h_g$ #4 | 790 | 0.17 | 0.25 | $h_g$ #4 | 790 | 0.00 | 0.00 | $h_g$ #4 |
| $a_g$ | 1114 | 0.05 | 0.14 | $h_g$ #5, $g_g$ #4 | 1113 | 0.09 | 0.26 | $h_g$ #5, $g_g$ #4 | 1114 | 0.13 | 0.38 | $h_g$ #5 |
| $a_g$ | 1124 | 2.01 | 6.11 | $g_g$ #4, $h_g$ #5 | 1123 | 2.06 | 6.16 | $h_g$ #5 | 1124 | 1.96 | 5.84 | $h_g$ #5 |
| $a_g$ | 1131 | 0.05 | 0.15 | $h_g$ #5, $g_g$ #4 | 1131 | 0.01 | 0.03 | $g_g$ #4, $h_g$ #5 | 1131 | 0.09 | 0.27 | $h_g$ #5, $g_g$ #4 |
| $a_g$ | 1271 | 0.56 | 2.17 | $h_g$ #6 | 1271 | 0.57 | 2.18 | $h_g$ #6 | 1271 | 0.59 | 2.24 | $h_g$ #6 |
| $a_g$ | 1278 | 0.06 | 0.23 | $h_g$ #6 | 1277 | 0.06 | 0.22 | $h_g$ #6 | 1277 | 0.08 | 0.32 | $h_g$ #6 |
| $a_g$ | 1332 | 0.02 | 0.07 | $g_g$ #5 | 1331 | 0.01 | 0.05 | $g_g$ #5 | 1331 | 0.01 | 0.04 | $g_g$ #5 |
| $a_g$ | 1447 | 0.20 | 0.99 | $h_g$ #7 | 1446 | 0.27 | 1.32 | $h_g$ #7 | 1447 | 0.26 | 1.30 | $h_g$ #7 |
| $a_g$ | 1460 | 4.69 | 24.06 | $h_g$ #7 | 1460 | 4.79 | 24.21 | $h_g$ #7 | 1460 | 4.86 | 24.53 | $h_g$ #7 |
| $a_g$ | 1510 | 0.04 | 0.23 | $a_g$ #2 | 1510 | 0.05 | 0.25 | $a_g$ #2 | 1510 | 0.05 | 0.26 | $a_g$ #2 |
| $a_g$ | 1519 | 0.00 | 0.03 | $g_g$ #6 | 1519 | 0.00 | 0.01 | $g_g$ #6 | 1519 | 0.00 | 0.00 | $g_g$ #6 |
| $a_g$ | 1583 | 2.06 | 12.38 | $h_g$ #8 | 1583 | 1.99 | 11.77 | $h_g$ #8 | 1584 | 2.11 | 12.55 | $h_g$ #8 |
| $a_g$ | 1589 | 1.20 | 7.33 | $h_g$ #8 | 1589 | 1.38 | 8.26 | $h_g$ #8 | 1589 | 1.25 | 7.49 | $h_g$ #8 |

**Table S4:** Analysis of the multimode JT problem of $C_{60}^{-}$ in $C_{2h}$ conformation by the LS totally symmetric modes in the harmonic approximation. Frequencies ($\nu_k$) of the selected normal modes are in $cm^{-1}$ as obtained from DFT calculations. The contributions of the normal mode to the JT distortion ($c_k$) and the energy stabilization ($E_k$) are given in %. The origin of the normal mode relative to the HS normal mode is given. The origin of the LS normal mode relative to the HS normal mode is given

| **LS irrep** | | | $^2$**A$_u$ (C$_{2h}$)** | | | | $^2$**B$_u$ (C$_{2h}$)** | |
|---|---|---|---|---|---|---|---|---|
| | $\nu_k$ | $c_k$ | $E_k$ | **Origin** | $\nu_k$ | $c_k$ | $E_k$ | **Origin** |
| $a_g$ | 261 | 7.14 | 1.19 | $h_g$ #1 | 27 | 0.06 | 0.00 | $h_g$ #1, $h_g$ #2 |
| $a_g$ | 263 | 0.32 | 0.05 | $h_g$ #1 | 263 | 0.17 | 0.03 | $h_g$ #1 |
| $a_g$ | 264 | 25.83 | 4.41 | $h_g$ #1 | 263 | 34.87 | 6.03 | $h_g$ #1 |
| $a_g$ | 424 | 29.96 | 13.23 | $h_g$ #2 | 297 | 0.39 | 0.09 | $h_g$ #1, $h_g$ #2 |
| $a_g$ | 433 | 8.73 | 4.02 | $h_g$ #2 | 425 | 34.70 | 15.66 | $h_g$ #2 |
| $a_g$ | 435 | 0.15 | 0.07 | $h_g$ #2 | 434 | 2.43 | 1.14 | $h_g$ #2 |
| $a_g$ | 482 | 0.00 | 0.00 | $g_g$ #1 | 480 | 0.02 | 0.01 | $g_g$ #1 |
| $a_g$ | 484 | 0.01 | 0.00 | $g_g$ #1 | 483 | 0.00 | 0.00 | $g_g$ #1 |
| $a_g$ | 500 | 0.40 | 0.24 | $a_g$ #1 | 500 | 0.27 | 0.17 | $a_g$ #1 |
| $a_g$ | 555 | 0.01 | 0.00 | $t_{2g}$ #1 | 553 | 0.00 | 0.00 | $g_g$ #2, $t_{2g}$ #1 |
| $a_g$ | 566 | 0.00 | 0.00 | $g_g$ #2, $t_{1g}$ #1 | 556 | 0.01 | 0.01 | $t_{2g}$ #1, $g_g$ #2 |
| $a_g$ | 571 | 0.00 | 0.00 | $g_g$ #2, $t_{1g}$ #1 | 570 | 0.00 | 0.00 | $t_{1g}$ #1 |
| $a_g$ | 577 | 0.00 | 0.00 | $g_g$ #2, $t_{1g}$ #1 | 573 | 0.01 | 0.00 | $h_g$ #3, $g_g$ #2 |
| $a_g$ | 707 | 0.66 | 0.81 | $h_g$ #3 | 573 | 0.00 | 0.00 | $g_g$ #2, $h_g$ #3 |
| $a_g$ | 707 | 3.64 | 4.48 | $h_g$ #3 | 707 | 0.61 | 0.76 | $h_g$ #3 |
| $a_g$ | 708 | 7.19 | 8.84 | $h_g$ #3 | 708 | 10.70 | 13.40 | $h_g$ #3 |
| $a_g$ | 754 | 0.01 | 0.01 | $t_{2g}$ #2 | 744 | 0.01 | 0.01 | $g_g$ #3 |
| $a_g$ | 759 | 0.00 | 0.00 | $g_g$ #3 | 756 | 0.01 | 0.01 | $g_g$ #3 |
| $a_g$ | 766 | 0.00 | 0.00 | $g_g$ #3, $t_{2g}$ #3 | 765 | 0.01 | 0.02 | $h_g$ #4, $t_{2g}$ #2, $t_{2g}$ #3 |
| $a_g$ | 787 | 4.79 | 7.28 | $h_g$ #4 | 766 | 0.00 | 0.00 | $t_{2g}$ #2, $h_g$ #4, $t_{2g}$ #3 |
| $a_g$ | 789 | 0.01 | 0.01 | $h_g$ #4 | 787 | 4.97 | 7.68 | $h_g$ #4 |
| $a_g$ | 789 | 0.22 | 0.33 | $h_g$ #4 | 789 | 0.01 | 0.02 | $h_g$ #4, $g_g$ #3 |
| $a_g$ | 801 | 0.00 | 0.00 | $t_{2g}$ #3, $g_g$ #3 | 801 | 0.00 | 0.00 | $t_{2g}$ #3 |
| $a_g$ | 831 | 0.00 | 0.00 | $t_{1g}$ #2 | 831 | 0.00 | 0.00 | $t_{1g}$ #2 |
| $a_g$ | 1114 | 0.11 | 0.34 | $h_g$ #5, $g_g$ #4 | 1022 | 0.00 | 0.00 | $g_g$ #4, $h_g$ #5 |
| $a_g$ | 1119 | 0.00 | 0.00 | $g_g$ #4, $h_g$ #5 | 1115 | 0.18 | 0.56 | $h_g$ #5 |
| $a_g$ | 1124 | 1.91 | 5.91 | $h_g$ #5, $g_g$ #4 | 1117 | 0.02 | 0.06 | $g_g$ #4, $h_g$ #5 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| $a_g$ | 1130 | 0.00 | 0.00 | $h_g$ #5, $g_g$ #4 | 1124 | 1.85 | 5.81 | $h_g$ #5, $g_g$ #4 |
| $a_g$ | 1131 | 0.05 | 0.14 | $h_g$ #5, $g_g$ #4 | 1130 | 0.01 | 0.02 | $h_g$ #5, $g_g$ #4 |
| $a_g$ | 1271 | 0.62 | 2.47 | $h_g$ #6 | 1201 | 0.01 | 0.04 | $h_g$ #6, $h_g$ #5, $g_g$ #4 |
| $a_g$ | 1277 | 0.06 | 0.24 | $h_g$ #6 | 1272 | 0.68 | 2.74 | $h_g$ #6 |
| $a_g$ | 1279 | 0.00 | 0.00 | $h_g$ #6 | 1279 | 0.02 | 0.07 | $h_g$ #6 |
| $a_g$ | 1290 | 0.00 | 0.00 | $t_{1g}$ #3 | 1301 | 0.00 | 0.00 | $t_{1g}$ #3 |
| $a_g$ | 1331 | 0.01 | 0.05 | $g_g$ #5 | 1311 | 0.00 | 0.00 | $h_g$ #6, $h_g$ #7, $t_{1g}$ #3 |
| $a_g$ | 1335 | 0.00 | 0.00 | $g_g$ #5 | 1327 | 0.01 | 0.05 | $g_g$ #5 |
| $a_g$ | 1357 | 0.00 | 0.00 | $t_{2g}$ #4 | 1334 | 0.00 | 0.01 | $g_g$ #5 |
| $a_g$ | 1447 | 0.17 | 0.85 | $h_g$ #7 | 1357 | 0.00 | 0.00 | $t_{2g}$ #4 |
| $a_g$ | 1451 | 0.00 | 0.00 | $h_g$ #7 | 1451 | 0.04 | 0.21 | $h_g$ #7 |
| $a_g$ | 1461 | 4.75 | 24.84 | $h_g$ #7 | 1461 | 4.73 | 25.20 | $h_g$ #7 |
| $a_g$ | 1510 | 0.00 | 0.02 | $a_g$ #2 | 1510 | 0.01 | 0.07 | $a_g$ #2 |
| $a_g$ | 1519 | 0.00 | 0.00 | $g_g$ #6 | 1518 | 0.00 | 0.00 | $g_g$ #6 |
| $a_g$ | 1520 | 0.00 | 0.02 | $g_g$ #6 | 1519 | 0.00 | 0.01 | $g_g$ #6 |
| $a_g$ | 1583 | 0.02 | 0.11 | $h_g$ #8 | 1539 | 0.00 | 0.03 | $h_g$ #8, $h_g$ #7 |
| $a_g$ | 1583 | 2.05 | 12.60 | $h_g$ #8 | 1583 | 0.68 | 4.27 | $h_g$ #8 |
| $a_g$ | 1589 | 1.19 | 7.40 | $h_g$ #8 | 1587 | 2.51 | 15.79 | $h_g$ #8 |